



chain nodes :

7 20 21 22 23 24 25 27

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16 17 18 19

chain bonds :

3-20 6-7 7-9 7-14 13-24 20-21 20-22 22-23 22-27 24-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13 14-15 14-19 15-16 16-17
17-18 18-19

exact/norm bonds :

13-24 14-15 14-19 15-16 16-17 17-18 18-19 20-21 20-22 24-25

exact bonds :

3-20 6-7 7-9 7-14 22-23 22-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

isolated ring systems :

containing 1 : 8 : 14 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS